The ***mar345*** Program Manual

Version 2.0

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Contents

1. Introduction

The program ***mar345*** is a fully menu driven graphical user interface (GUI) for collecting and displaying images on a ***mar345*** imaging plate system.

The program is provided as binary executable for several computer platforms and operating systems:

- **Silicon Graphics**: IRIX 5.x, 6.x
- **Digital**: Compaq Tru Unix 4.x, 5.x
- **Linux**: RedHat 5.x, 6.x, SuSE 6.x

1.1 Computer Requirements

- Motif 1.2.x shared libraries (except Linux).
- 8/16/24/32-bit colors X-windows terminal with 1280x1024 pixels.
- Standard Helvetica and Symbol fonts.
- 96 MB RAM memory or more.

1.2 Environment

The program relies on definitions of the following environment variables:

- **MARTABLEDIR** Location of the scanner specific calibration files **mar2300.XXX** and **mar3450.XXX** and the corresponding configuration file **config.XXX** (where XXX = MAR_SCANNER_NO).
- **MAR_SCANNER_NO** Three digit serial number, e.g. 049.
- **MARLOGDIR** Location of the log output files.
- **MARHELPDIR** Location of interactive help files.

The program relies on the correct network setup, i.e. the **mar345** scanner must be accessible by **ping** and **telnet** with IP-address 192.0.2.1.

For a description of the setup of the ***mar345*** software suite, see the "***mar345 Installation Guide***".

2. Running *mar345*

2.1 Command Line

The program ***mar345*** should be started by just typing "*mar345*". The program, however, understands the following command line options:

mar345 [-h] [-colors N] [-def YYYY] [-host HOST] [-keep]

[-more N] [-noxf] [-port PORT] [-setd]

The command line options are:

-h	Print a usage summary
-colors N	Use N colors for drawing images. **Default**: take N from configuration file.
-def XXXX	When starting the program, go to scanmode XXXX where XXXX is 1200, 1600, 1800, 2000, 2300, 2400, 3000 or 3450. **Default**: stay in current scan mode.
-host HOST	Connect to host HOST. **Default**: take HOST from configuration file (usually 192.0.2.1)
-keep	Spiral images will be saved on disk. **Default**: do not produce spiral files, only transformed images.
-more N	Log output level with N=0, 1, 2 or 3. Use more > 0 only in case of hardware problems. **Default**: N=0 (compact output)
-noxf	Spiral images will not be transformed into Cartesian images. The program then requires much less memory, but images cannot be displayed. **Default**: Do transform spiral images.
-port PORT	Connect to host HOST via socket port PORT

2.2 Input Files

The program ***mar345*** requires the following input files to work properly:

The program continuously saves edited parameters into this file. It is nice to find the program

The contents of the different types of log files are as follows:

1.) **mar.log:** All messages on the terminal output.

2.) **mar.spy:** Native mar345 controller messages

These messages become very important in case of hardware problems. Therefore, **USE SPY** should always be set.
Note, that these files can become very large in size, so sufficient disk space should be available in $MARLOGDIR (up to 100 MB in total).

3.) **mar.lp:** Some image statistics like minimum, maximum and average intensity. Normally, these values are not of much interest, so **USE STATS** should rather be the exception.

2.4 Basic Concepts and Rules

The program has to perform different tasks:

- Allow user input (i.e. change data collection parameters, analyze images, etc.)
- Send commands to the scanner.
- Receive information from the scanner

2.5 Starting Up

Create a new window for running the program and type: "*mar345*". Do not run the program in the background and do not use this window for other purposes. The program will send important output to the window and you don't want to miss it.
At start up, the program will tell you something like:

```
Program      :  mar345
Version      :  2.0.8 (Feb 16 2000)
Scanner no.  :  049
Scanner mode:  345 mm @ 0.15 mm
Started on   :  Wed Feb 16 15:09:08 2000
LOG  file is:  /home/mar345/log/log/mar.log.58
SPY  file is:  /home/mar345/log/spy/mar.spy.58
STAT file is:  /home/mar345/log/lp/mar.lp.58
```

It will also tell you if it is able to talk to the scanner. If environment variables are not set you will be notified. Next, three windows will be created and automatically placed on the screen: a startup window, the mar345 main window and an empty image display window.

If the scanner is not turned on at all, by invoking program mar345 on the command line, you will not get any feed back. This is because the program tries to open a network connection to the scanner and the program will sit there and wait until the scanner starts talking to it.

When the scanner is turned on, the scanner controller will start very quickly basic network services, so a ping to the address of the scanner (usually 192.0.2.1) will work within 10 seconds after turning the scanner on. However, before starting communication with the program mar345, the scanner must do first some initialization, i.e. drive the scanning head to

The main window controls the most important scanner functions. It consists of different areas:

- a menu bar
- the scanner status area
- the scanner command area

3.2 Menu Bar

The menu bar features two buttons:

Windows Pops up the ***Windows*** submenu (3.2.1).
Shortcut: **Alt+w**.

Help Pops up the ***mar345-Help*** window.
Shortcut: **F5**.

3.2.1 Windows Submenu

The Windows submenu pops up if the "Windows" button in the menu bar was pressed or if **"Alt+w"** was pressed while the pointer was in the main window.

Move Distance	Pops up the ***mar345–Distance*** window. Shortcut: **F8.**
Move Phi	Pops up the ***mar345–Phi*** window. Shortcut: **F9.**
Reset Scanner	Reboots the scanner reboot. Shortcut: **Ctrl+r.**
Quit	Quits program. Shortcut: **Ctrl+q.**

3.3 Scanner Status Area

Note: Timing is a crucial issue when operating the scanner. If the computer is very busy doing other computations, the internal clock of the program will work slower. A good check for excessive computer activity is if the X-windows server is not able to repaint the user interace at a reasonable speed.

3.4 Scanner Command Area

The buttons in the command area can be used to send commands directly to the scanner or

to pop up further windows, i.e. the ***mar345-Scan*** and ***mar345-Change Parameters*** windows. The functions of the individual buttons are:

Button	Description
Collect	Changes layout of the button choices, i.e. the ***Collect Menu*** buttons are displayed.
Scan	Pops up the ***mar345-Scan*** window.
Erase	Immediately starts to erase the imaging plate. Erasing is identical to doing a scan, but no data are taken.
Initialize	The scanner will move to its distance reference position (usually at the far end

The ***Change Parameters*** window is used to program data collection parameters. The window comes in 4 slightly different flavours, depending on the button choice in the ***Collect Menu***:

– Single Data Set

– Index Crystal

The difference is, that in **Multiple Data Sets** one can program up to 64 data sets with the full range of parameters. The amount of data sets that are offered for programming can be

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Item	Description
First image no.	Image number of first image. Range is 1 through 999.
No. of images	Number of images to be collected. Range is 1 through 999.

may be different from the desired exposure time.

Oscillations	Number of φ–oscillations per image. One oscillation is

3.6 Loading and Saving Data Collection Parameters

Crystallographers often collect data of a certain crystal type in always the same way, i.e. using a certain oscillation range, a certain distance, etc. It is therefore useful to store a typical set of data collection parameters to a file and retrieve the parameters when desired. To save parameters, press the "**Save**" button in the ***mar345–Change Parameters*** window.

[redacted]

mar345–Change Parameters window. It is a good idea to always let the plate clean first

[redacted]

3.12 Getting Help

Interactive help can be obtained by

3.14 X-ray Setup

When producing images during data collection many parameters concerning the current experiment are automatically written into the output image headers, so this information can be retrieved later on. This is most relevant for parameters like the distance and the goniometer positions. It might, however, be useful to add also some information about the state of the X-ray source. Unfortunately, the program ***mar345*** does not have knowledge about the generator and collimator settings, so this information must be entered manually. For this purpose, open the ***mar345 X-ray Setup*** window. This window can be popped up

During operation, i.e. data collection or other tasks, the scanner itself or the program ***mar345*** might produce error messages or warnings. All relevant messages are displayed automatically in the ***mar345 Error*** window. This window can be popped up manually from the main window menubar or by pressing the **F7** key. Some warnings and errors may have an obvious solution if they are not related to the scanner hardware. For latter ones, please

The menu bar features the following buttons:

Windows Pops up the ***Windows*** submenu (see 4.2.1). Shortcut: **Alt+w**.

Options Pops up the ***Options*** submenu (see 4.2.2). Shortcut: **Alt+o**.

Help Pops up the ***mar345−Help*** window.

4.2.1 Windows Submenu

The Windows submenu pops up when the "**Windows**" button in the menu bar was pressed or if **"Alt+w"** was pressed while the pointer was in the main window. The submenu is a so called "tear−off" menu.

The Windows menu features the following buttons:

Files Pops up the ***mar345−Files*** window

Do not/Keep color scales Normally, if a new image is loaded, the program recalculates a new color scheme. If you want all images to be displayed

Reset colors Recalculates colors and redisplays the image.
Shortcut: **Ctrl+t**

Turn On/Off 3D-plot Toggles 3-D representation of magnified areas of the image. Available only at zoom factors > 4.
Shortcut: **Ctrl+d**

Next image Load the next image, i.e. increment image number by 1.

4.3 Image Area

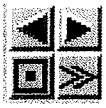
In this area, the image is displayed. With the pointer (3-way mouse button) several additional functions can be accessed.

Button	Action	Result
Left	**Press**	Pops up an empty ***mar345-Cross section*** window
	Drag	A red line is drawn from the position of the first mouse press to the position of the last mouse press.
	Release	The (interpolated) intensities of the pixels along the line are displayed in the ***mar345-Cross section*** window.
Center	**Press**	The x,y-coordinate, intensity and resolution of the pixel is displayed in the information area in the upper left corner of the image area.

The right mouse button functions depend on the current zoom factor. At **zoom factors < 1**, the behaviour is as follows:

Button	Action	Result

4.4.1 Load Buttons



By pressing the single left or right arrow one can decrease or increase the current image number and load the previous or next image, respectively. The double arrow will continously increase image numbers and continuously load the next image until the stop button is pressed.

The functions of the ***mar345-Colors*** window widgets are:

Grey scales Selection of coloring mode. Alternatives: **Blue scales, Rainbow**.

Min All pixels with intensities <= Min are drawn white (black in Blue scales). The dashed line in the histogram plot moves to the specified value.

Max All pixels with intensities >= Max are drawn black (Grey scales), white (Blue scales) or red (Rainbow). Intensities which are above the saturation limit (128000) are drawn in green. The dashed line in the histogram plot moves to the specified value.

In the histogram plot, the mouse buttons have the following functions:

Left mouse button press Places the dashed red line in the histogram plot to a new position marking the minimum. The value in the "**Min**" text field is changed accordingly.

Right mouse button press Places the dashed red line in the histogram plot to a new position marking the maximum. The value in the "**Max**" text field is changed accordingly.

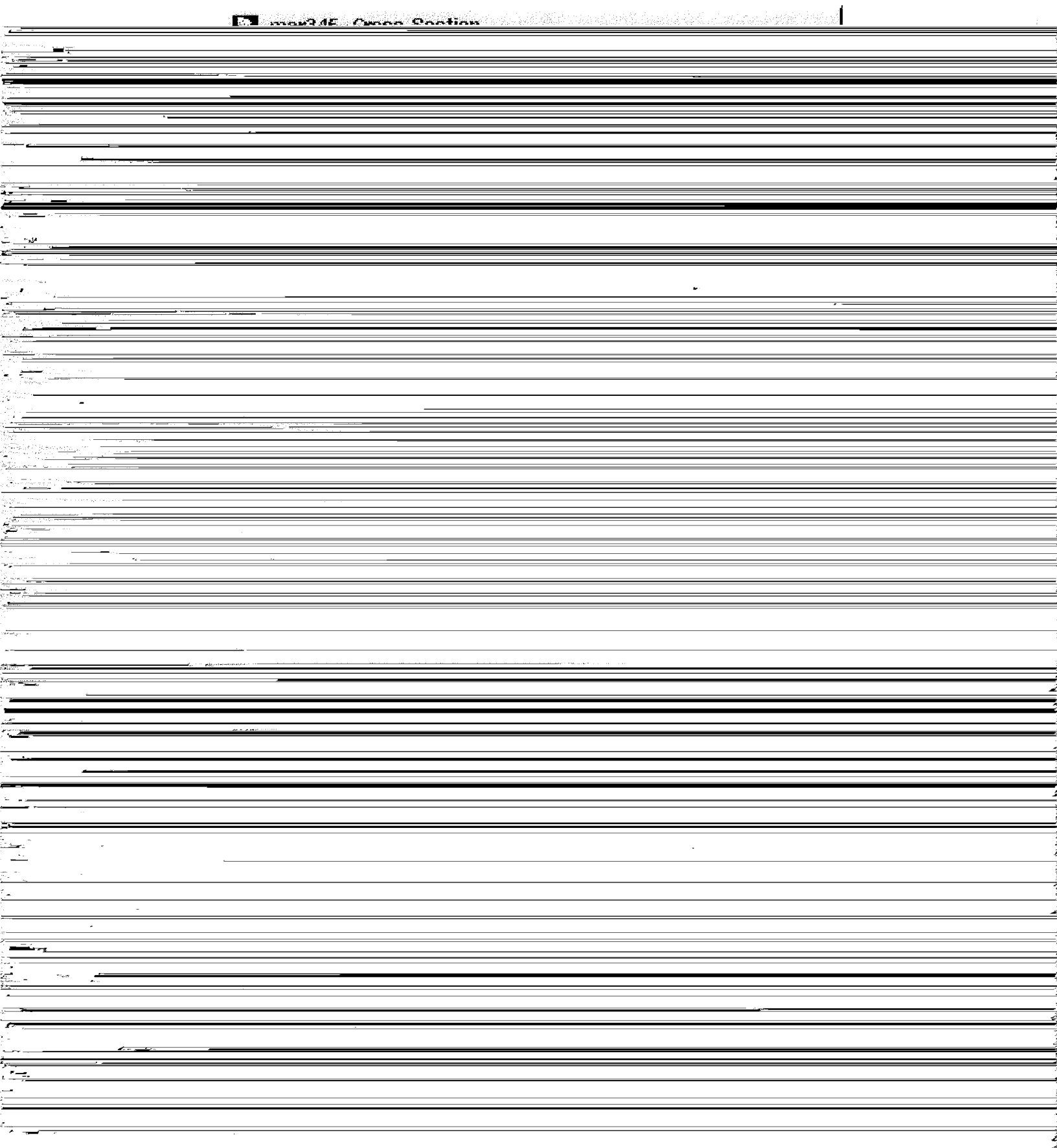
Center mouse button drag Changes color tables. Try it out to see what it really does. This

works for grey and blue scales only and for 8-bit color displays

only!

Note:
By changing **Min** or **Max** or setting these values with the mouse button the color distribution for the whole image will be recalculated. This takes some CPU-time, so please don't do

4.8 Cross-Section Window



The **plot area** of the window shows the following features:

Vertical axis Interpolated intensities

Upper horizontal axis Length of line in pixel units.

Lower horizontal axis Length of line in mm units.

Left dashed red line Marks the begginning of a measured distance. This line can be moved using the **left mouse button**.

Right dashed red line Marks the begginning of a measured distance. This line can be moved using the **right mouse button**.

Horizontal red lines Shows the length of the line in pixels (mm) and the distance between the dashed vertical lines.

The pointer can be used to measure distances by setting the red dashed lines to the desired positions on the drawn line. This is particularly useful if you want to measure all separations

5. Data Collection

5.1 Strategies

While some general rules apply how to collect data best, a sensible choice of data collection parameters depends on individual circumstances, i.e. crystal quality, beam properties, etc.

The decision about what pixelsize to choose is slightly more difficult. In general, the finest pixelsize of 0.1mm is more efficient and yields slightly better data. On the other hand, scans take about 10% longer time and images are larger in size than those taken at the same

diameter but in 0.15mm pixelsize mode. So the decision is some kind of compromise.

Output format:
Use of "mar345" format is strongly suggested. A mar345 file typically requires 70% less disk space than a standard uncompressed image file. All major protein data processing packages

Collect mode:
Use TIME mode unless on synchrotrons.

[redacted]

[redacted]

Both the computer and the scanner can produce fatal errors and warnings. All messages are

[redacted]

numbered. Messages with message numbers < 1000 come directly from the scanner

[redacted]

Tabel continued from previous page.

1050 **Message:** "SHUTTER did not work properly. Abandoning data collection"
Reason: X-ray beam shutter damaged or dirty.

to operate?

1060 **Message:** "X-ray reading too low "

Reason: The X-ray intensity as read from the ion. chamber is below the critical level (see configuration file: INTENSITY MIN xxx). The data collection starts only if the X-ray reading is above the configured value.

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No.	Description	
1101	**Message:**	"No scan modes found in nb_code ..."
1102		"Something wrong with byteorder in nb_code ..."
1105		"No suitable scanning mode found in nb_code".
	Reason:	File $MARTABLEDIR/mar2300.XXX and/or $MARTABLEDIR/mar3450.XXX may be corrupted or empty.
	Action:	Check file sizes (73 MB and 103MB). Use command: catmar $MARTABLEDIR/mar2300.XXX to look at the calibration file header.
1103	**Message:**	"Scanner serial number in nb_code differs from config"
	Reason:	The scanner no. in the file headers of files $MARTABLEDIR/mar2300.XXX and/or $MARTABLEDIR/mar3450.XXX are not identical to $MAR_SCANNER_NO. The calibration files may not belong to the scanner.
	Action:	Call.
1110	**Message:**	"Cannot create image file"
1111		"Cannot open image file"
1112		"Error writing image array"
1115		"Error writing image header"
	Reason:	[redacted]

Appendix

A. Configuration File

Each scanner has a scanner specific configuration file. This file must reside in directory

B. Calibration Files

Each scanner comes with 2 scanner specific calibration files. These files must reside in directory $MARTABLEDIR and are called mar2300.XXX and mar3450.XXX, where XXX is the three-digit serial number. The file contain flat field and geometrical corrections required for producing Cartesian images out of a spiral scan.

- File mar2300.XXX is used for scans at pixelsizes of 0.15mm (modes 2300, 2000, 1600 and 1200) and has a typical size of 73 MB